Nomenclature of Tetrapyrroles

Continued from Appendix 1

Appendix 2 and 3

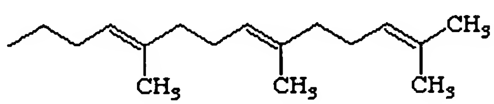
Contents

Appendix 2

Comparison of the Numbering of the Trivially Named Porphyrins(TNP) with Numbering Based on CNOC/CAS

TNP Trivial Name	**Numbering Basis**	2	3	7	8	12	13	15	17	18	20
1. Uroporphyrin I	TNP	Cm	Cet	Cm	Cet	Cm	Cet	-	Cm	Cet	-
	CNOC/CAS	Cet	Cm	Cet	Cm	Cet	Cm	-	Cet	Cm	-
2. Coproporphyrin II	TNP	Me	Cet	Cet	Me	Me	Cet	-	Cet	Me	-
	CNOC/CAS	Cet	Me	Me	Cet	Cet	Me	-	Me	Cet	-
3. Etioporphyrin I	TNP	Me	Et	Me	Et	Me	Et	-	Me	Et	-
	CNOC/CAS	Et	Me	Et	Me	Et	Me	-	Et	Me	-
4. Etioporphyrin II	TNP	Me	Et	Et	Me	Me	Et	-	Et	Me	-
	CNOC/CAS	Et	Me	Me	Et	Et	Me	-	Me	Et	-
5. Etioporphyrin III	TNP	Me	Et	Me	Et	Me	Et	-	Et	Me	-
	CNOC/CAS	Et	Me	Et	Me	Et	Me	-	Me	Et	-
6. Etioporphyrin IV	TNP	Me	Et	Me	Et	Et	Me	-	Et	Me	-
	CNOC/CAS	Et	Me	Et	Me	Me	Et	-	Me	Et	-
7. Cytoporphyrin	TNP	Me	$R^1CH(OH)$-	Me	Vn	Me	Cet	-	Cet	-CHO	-
	CNOC/CAS	Cet	Me	Vn	Me	$R^1CH(OH)$-	Me	-	-CHO	Cet	-

8. Protoporphyrin	TNP	Me	Vn	Me	Vn	Me	Cet	-	Cet	Me	-
	CNOC/CAS	Cet	Me	Vn	Me	Vn	Me	-	Me	Cet	-
9. Mesoporphyrin	TNP	Me	Et	Me	Et	Me	Cet	-	Cet	Me	-
	CNOC/CAS	Cet	Me	Et	Me	Et	Me	-	Me	Cet	-
10. Hematoporphyrin	TNP	Me	$CH_3CH(OH)$-	Me	$CH_3CH(OH)$-	Me	Cet	-	Cet	Me	-
	CNOC/CAS	Cet	Me	$CH_3CH(OH)$-	Me	$CH_3CH(OH)$-	Me	-	Me	Cet	-
11. Deuteroporphyrin	TNP	Me	-	Me	-	Me	Cet	-	Cet	Me	-
	CNOC/CAS	Cet	Me	Me	-	Me	-	-	Me	Cet	-
12. Rhodoporphyrin	TNP	Me	Et	Me	Et	Me	-COOH	-	Cet	Me	-
	CNOC/CAS	Cet	Me	Me	Et	Me	Et	-	Me	-COOH	-
13. Pyrroporphyrin	TNP	Me	Et	Me	Et	Me	-	-	Cet	Me	-
	CNOC/CAS	Cet	Me	Me	Et	Me	Et	-	Me	-	-
14. Phylloporphyrin	TNP	Me	Et	Me	Et	Me	-	Me	Cet	Me	-
	CNOC/CAS	Cet	Me	Me	Et	Me	Et	-	Me	-	Me

R^1 = 

Cm = $-CH_2COOH$

Cet = $-CH_2CH_2COOH$

CNOC = IUPAC Commission on Nomenclature of Organic Chemistry

CAS = Chemical Abstracts Service

Note: Cet and Cm are often abbreviated to P and A. This is acceptable provided these are defined as $CH_2CH_2CO_2H$ and CH_2CO_2H respectively.

Appendix 3

Fischer trivial names

App No.: 10/812,156 Docket No.: 606952000420
Inventor: Robert A. VUKOVICH et al.
Title: PREPARATION OF METAL MESOPORPHYRIN COMPOUNDS
Exhibit 1 - Page 3 of 5

The following extensions to the list of accepted trivial names are proposed as permitted: they encompass a further selection of trivial names due to Hans Fischer. They each refer to a single compound and must not be used as a basis for semisystematic nomenclature.

A. Porphyrins

The names are illustrated for isomers of mesoporphyrin, but may also be used for deuteroporphyrin (for Et read H), haematoporphyrin (for Et read -CH(OH)CH_3) and protoporphyrin (for Et read -CH=CH_2).

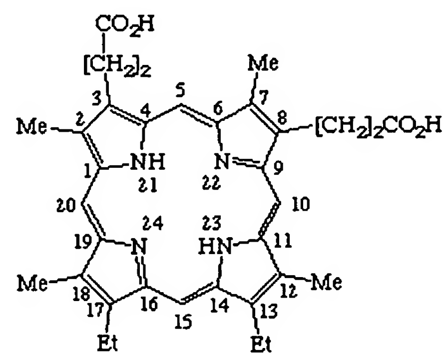
The names all carry a Roman numeral. The name without such a numeral is already defined in Table 2, and corresponds to isomer IX in the Fischer scheme. The Roman numerals here do **not** mean the same as those employed in the trivial names in Table 3. Both systems are referred to as "type numbering". The start point and sequence of locant numbering used by Fischer are retained (although the locant numbers follow the 1-24 system, TP-1.2).

Comparison of the Numbering of the Fischer Trivially Named Porphyrins (TNP) with Numbering Based on CNOC/CAS Numbering Principles. Cm = -CH_2COOH; Cet = -CH_2CH_2COOH; CNOC = IUPAC Commission on the Nomenclature of Organic Chemistry; CAS = Chemical Abstracts Service.

Fischer Isomer Type Number	Numbering Basis	Substituents and Locants							
		2	3	7	8	12	13	17	18
I	TNP	Me	Et	Me	Et	Me	Cet	Me	Cet
	CNOC/CAS	Cet	Me	Cet	Me	Et	Me	Et	Me
II	TNP	Me	Cet	Me	Et	Me	Cet	Me	Et
	CNOC/CAS	Cet	Me	Et	Me	Cet	Me	Et	Me
III	TNP	Me	Et	Et	Me	Me	Cet	Cet	Me
	CNOC/CAS	Cet	Me	Me	Et	Et	Me	Me	Cet
IV	TNP	Me	Cet	Et	Me	Me	Et	Cet	Me
	CNOC/CAS	Cet	Me	Me	Cet	Et	Me	Me	Et
V	TNP	Me	Cet	Et	Me	Me	Cet	Et	Me
	CNOC/CAS	Cet	Me	Me	Et	Cet	Me	Me	Et
VI	TNP	Me	Cet	Me	Cet	Me	Et	Et	Me
	CNOC/CAS	Cet	Me	Cet	Me	Me	Et	Et	Me
VII	TNP	Me	Cet	Me	Et	Me	Cet	Et	Me
	CNOC/CAS	Cet	Me	Et	Me	Cet	Me	Me	Et

VIII	TNP	Me	Et	Me	Cet	Me	Cet	Et	Me
	CNOC/CAS	Cet	Me	Cet	Me	Et	Me	Me	Et
IX	TNP	Me	Et	Me	Et	Me	Cet	Cet	Me
	CNOC/CAS	Cet	Me	Et	Me	Et	Me	Me	Cet
X	TNP	Me	Et	Me	Cet	Me	Et	Cet	Me
	CNOC/CAS	Cet	Me	Et	Me	Me	Cet	Et	Me
XI	TNP	Me	Cet	Me	Et	Me	Et	Cet	Me
	CNOC/CAS	Cet	Me	Me	Cet	Et	Me	Et	Me
XII	TNP	Me	Et	Et	Me	Cet	Me	Me	Cet
	CNOC/CAS	Cet	Me	Me	Cet	Me	Et	Et	Me
XIII	TNP	Et	Me	Me	Et	Me	Cet	Cet	Me
	CNOC/CAS	Cet	Me	Et	Me	Me	Et	Me	Cet
XIV	TNP	Me	Cet	Et	Me	Et	Me	Me	Cet
	CNOC/CAS	Cet	Me	Cet	Me	Me	Et	Me	Et
XV	TNP	Me	Cet	Et	Me	Cet	Me	Me	Et
	CNOC/CAS	Cet	Me	Et	Me	Me	Cet	Et	Me

Thus mesoporphyrin VI is



B. Bilindiones

The following Fischer trivial names for bile pigments are permitted. Each refers to a single compound, and must not be used as the basis for semisystematic nomenclature. They each have a Roman numeral and a Greek letter as suffixes: the Roman numeral refers to the porphyrin structure (tabulated above) which has been formally broken at the meso bridge denoted by the Greek letter (Fischer numeration, Fig. 1). The structures and names have already been referred to in TP-6.3 and TP-6.4 and are:

biliverdin IIIα, biliverdin IXα (= biliverdin), biliverdin IXβ, biliverdin IXγ, biliverdin IXδ, biliverdin XIIIα, together with the corresponding hydrogenated derivatives (e.g. bilirubins, mesobiliverdins).

The names without a Roman numeral and Greek letter are already defined in Fig. 16-22: in each case the IXα isomer is implied. For convenience the structures of the biliverdin isomers mentioned in the previous paragraph are tabulated below.

Roman Numeral Designation	Substituents at Positions							
	2	3	7	8	12	13	17	18
IXα	Me	Vn	Me	Cet	Cet	Me	Me	Vn
IXβ	Me	Cet	Cet	Me	Me	Vn	Me	Vn
IXγ	Cet	Me	Me	Vn	Me	Vn	Me	Cet
IXδ	Me	Vn	Me	Vn	Me	Cet	Cet	Me
IIIα	Vn	Me	Me	Cet	Cet	Me	Me	Vn
XIIIα	Me	Vn	Me	Cet	Cet	Me	Vn	Me

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come upon one such trend in Chapter 10: the general tendency for ionization energy to increase along any row of the periodic table. Our discussion in this and subsequent chapters will reveal other similar *horizontal* trends in chemical and physical properties. In addition, important *diagonal* relationships appear: There are often similarities between an element and its diagonal neighbor in the succeeding *column* and *row* of the periodic table. To make the existence of such relationships clear, and to emphasize the usefulness of the periodic table, in the remainder of this chapter we shall discuss some of the clearer trends in the properties of the elements and of some of their common compounds.

13.2 PERIODIC PROPERTIES

A very large number of chemical and physical properties of the elements vary periodically with atomic number. Some of these properties are related to the electron configurations of the atoms in quite obscure and complicated ways, while others are more susceptible to interpretation and explanation. These latter properties, such as electrical conductivity, crystal structure, ionization energy, electron affinity, possible oxidation states, and atomic size, are related to each other and to the general chemical behavior of the elements. Thus an appreciation of the importance of these particular properties, and of how they vary throughout the periodic table, will help us to correlate, remember, and predict the detailed chemistry of the elements.

Electrical and Structural Properties

The chemical elements can be classified as *metals*, *nonmetals*, and *semimetals* on the basis of their electrical properties alone. Metals are good conductors of electricity, and their electrical conductivity *decreases* slowly as temperature is increased. The nonmetals are electrical insulators: Their ability to conduct electricity is either extremely small or undetectable. The electrical conductivities of semimetals or semiconductors are small but measurable, and tend to *increase* as temperature increases. Electrical conductivities are usually measured in units of $ohm^{-1} \cdot cm^{-1}$, and a conductivity of $1\ ohm^{-1} \cdot cm^{-1}$ means that if a potential difference of 1 volt is applied to opposite faces of a 1-cm cube of material, a current of 1 amp will flow. The electrical conductivities of metals are, in general, greater than approximately $1 \times 10^4\ ohm^{-1} \cdot cm^{-1}$, as Table 13.2 shows. The shaded group of semimetals have small conductivities (in the range from 10 to $10^{-5}\ ohm^{-1} \cdot cm^{-1}$) that are sensitive to impurities, and nonmetals have even smaller conductivities (i.e., are insulators).

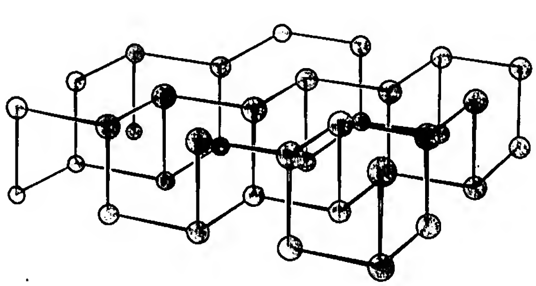
Table 13.2 shows that the metallic elements appear in the left-hand part of the periodic table, and are separated from the nonmetals by a *diagonal* band of semimetals that runs from boron to tellurium. The classification of elements close to this group of semimetals is not always straightforward, for several of the elements of groups IVA, VA, and VIA occur in different allotropic forms,

Table 13.2 The electrical conductivities of the elements in units of 10^4 ohms^{-1} · cm^{-1}

Li 11.8	Be 18		C	N	O	F
Na 23	Mg 25	Al 40		P	S	Cl
K 15.9	Ca 23	Ga 2.4			Se	Br
Rb 8.6	Sr 3.3	In 12	Sn 10	Sb 2.8		I
Cs 5.6	Ba 1.7	Tl 7.1	Pb 5.2	Bi 1.0	Po	At

Sc —	Ti 1.2	V 0.6	Cr 6.5	Mn 20	Fe 11.2	Co 16	Ni 16	Cu 65	Zn 18
Y —	Zr 2.4	Nb —	Mo 23	Tc —	Ru 8.5	Rh 22	Pd 1	Ag 66	Cd 15
La 1.7	Hf 3.4	Ta 7.2	W 20	Re —	Os 11	Ir 20	Pt 10	Au 49	Hg 4.4

each of which has different electrical properties. For example, the α-phase of tin, sometimes called grey tin, has the diamond type of crystal lattice found in silicon and germanium, and like these elements, grey tin has the electrical properties of a semimetal. On the other hand, white tin, the β-phase that is stable above 13°C, is a metallic conductor. As another example, white phosphorus, a molecular solid of P_4 units, and red phosphorus, which has a complex chain structure, are both electrical insulators and thus are of nonmetallic character. In contrast, the allotrope black phosphorus has a crystal structure made up of corrugated sheets, as shown in Fig. 13.2, and in this form phosphorus behaves like a semimetal. Similar phenomena are found for selenium.



The crystal structure of the black phosphorus allotrope. **FIG. 13.2**